LBN

MET O 11 TECHNICAL NOTE NO 85

# The change in the solution vector of a set of equations of condition when the equations are subject to a perturbation

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## 1. Introduction

Data fitting by least-squares is a technique having many applications in meteorology. It often happens that when one such problem has been solved and a solution vector obtained what is virtually the same problem has to be solved again with minor but significant changes in the equations of condition. It may be that part of the data vector is different, or some of the base functions are changed, or that the base functions remain the same but that some of the points at which they have to be evaluated are different. An example is provided by the optimal interpolation scheme of analysis. If a preferred list of stations is used around a grid point, or if the list of stations used in determined by some strong selection criterion, then the equations of conditions for determining the optimum weights may be quite similar from case to case, but experience shows that the differences cannot be ignored. Other examples will spring to mind.

This note explores the relationship between the solution vector of a system of equations of condition and the solution vector of the same system subject to a fairly general perturbation. An expression for the difference in the solution vectors is obtained.

N.B. This paper has not been published. Permission to quote from it must be obtained from the Assistant Director of the above Meteorological Office Branch.

## 2. Theory

Given a data set $h_1, h_2, ---, h_m$ at the discrete positions $x_1, x_2, ---, x_m$ we represent this data set by an analytical model of the form

$$\underset{m1}{\underline{h}} = a_1 \underset{m1}{\underline{f_1}} + a_2 \underset{m1}{\underline{f_2}} + ----- + a_n \underset{m1}{\underline{f_n}} + \underset{m1}{\underline{r}} \qquad (1)$$

where $\underline{h}$ is the m-vector $\underline{h} = \underline{h}(h_1, h_2, ---, h_m)$

$\underline{f}_i$ are the m-vectors $\underline{f}_i = \underline{f}_i (f_{1i}, f_{2i}, --- f_{mi})$, namely the evaluations of the i-th base function over the discrete domain, and $\underline{r}$ is the m-vector of residuals.

The model (1) may be rewritten as

$$\underset{m1}{\underline{h}} = \underset{mn}{F} \cdot \underset{n1}{\underline{a}} + \underset{m1}{\underline{r}} \qquad (2)$$

where $\underline{a}$ is the n-vector $\underline{a} = (a_1, a_2, ---, a_n)$

and F is the m x n matrix of column vectors $(\underline{f}_1 \mid \underline{f}_2 \mid \underline{f}_3 \mid ----- \mid \underline{f}_n)$

To make the matter specifically clear if the base functions are the set of monomials $(1, x, x^2, x^3)$ and the discrete domain is the set of points $(x_1, x_2, x_3, x_4, x_5)$ then the F matrix is, for example

$$\underset{54}{F} = \begin{pmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ 1 & x_3 & x_3^2 & x_3^3 \\ 1 & x_4 & x_4^2 & x_4^3 \\ 1 & x_5 & x_6^2 & x_5^4 \end{pmatrix} \qquad (3)$$

The fact that a polynomial example has been used here does not mean that what follows applies only to polynomial fitting. The $f_i$ may be any analytical functions.

The vector equation (2) thus represents m equations of condition. If different weights are given to each of these m equations on whatsoever grounds then this is catered for by introducing a diagonal weighting matrix into (2) so that it takes the form

$$\underset{mm}{W^{\frac{1}{2}}} \cdot \underset{mn}{F} \cdot \underset{n1}{\underline{a}} = \underset{mm}{W^{\frac{1}{2}}} \cdot \underset{m1}{\underline{h}} + \underset{mm}{W^{\frac{1}{2}}} \cdot \underset{m1}{\underline{r}} \qquad (4)$$

and it is in this form that we consider the problem.

The least-squares estimate $\hat{\underline{a}}$ of the coefficient vector $\underline{a}$ in (4) is given by the Normal Equations

$$\underset{nm}{(\tilde{F}} \cdot \underset{mm}{W} \cdot \underset{mn}{F)} \cdot \underset{n1}{\hat{\underline{a}}} = \underset{nm}{\tilde{F}} \cdot \underset{mm}{W} \cdot \underset{m1}{\underline{h}} \qquad (5)$$

which we will rewrite as

$$\underset{nn}{Q} \cdot \underset{n1}{\hat{\underline{a}}} = \underset{n1}{\underline{\ell}} \qquad (6)$$

Assume that in (4), $W$, F and $\underline{h}$ are changed to $\overset{*}{W}$, $\overset{*}{F}$, and $\overset{*}{\underline{h}}$. In place of (4) we then have

$$\overset{*}{W}^{\frac{1}{2}} \cdot \overset{*}{F} \cdot \underline{a} = \overset{*}{W}^{\frac{1}{2}} \cdot \overset{*}{\underline{h}} + \overset{*}{W}^{\frac{1}{2}} \cdot \underline{t} \tag{7}$$

with Normal Equations

$$\overset{*}{Q} \cdot \hat{\underline{a}} = \overset{*}{\underline{\ell}} \tag{8}$$

Define

$$\delta\hat{\underline{a}} = \hat{\underline{a}} - \hat{\underline{a}} \tag{9}$$

$$\delta\underline{\ell} = \overset{*}{\underline{\ell}} - \underline{\ell} \tag{10}$$

$$\delta Q = \overset{*}{Q} - Q \tag{11}$$

Putting (9) and (11) into (8) and subtracting (6) we get

$$\delta Q \cdot \hat{\underline{a}} + Q \cdot \delta\hat{\underline{a}} + \delta Q \cdot \delta\hat{\underline{a}} = \delta\underline{\ell} \tag{12}$$

which using (11) again, rearranges as

$$\delta\hat{\underline{a}} = \overset{*}{Q}^{-1} \cdot (\delta\underline{\ell} - \delta Q \cdot \hat{\underline{a}}) \tag{13}$$

and it can be similarly shown that

$$\delta\hat{\underline{a}} = Q^{-1} \cdot (\delta\underline{\ell} - \delta Q \cdot \hat{\underline{a}}) \tag{14}$$

Now assume that the models (4) and (7) are not totally different, but that some or most functions, data values and positions are the same in both cases. We can then write the matrices in (4) and (7) in partitioned form. Thus in (4)

$$W^{\frac{1}{2}} \cdot F = \begin{pmatrix} W^{\frac{1}{2}}_{ss} & 0_{s(m-s)} \\ \hline 0_{(m-s)s} & \omega^{\frac{1}{2}}_{(m-s)(m-s)} \end{pmatrix} \cdot \begin{pmatrix} A_{st} & \beta_{s(n-t)} \\ \hline \gamma_{(m-s)t} & \alpha_{(m-s)(n-t)} \end{pmatrix} = \begin{pmatrix} W^{\frac{1}{2}} \cdot A & W^{\frac{1}{2}} \cdot \beta \\ \hline \omega^{\frac{1}{2}} \cdot \gamma & \omega^{\frac{1}{2}} \cdot \alpha \end{pmatrix} \tag{15}$$

and

$$W^{\frac{1}{2}} \cdot \underline{h} = \begin{pmatrix} W^{\frac{1}{2}} & 0 \\ \hline 0 & \omega^{\frac{1}{2}} \end{pmatrix} \cdot \begin{pmatrix} \underline{c}_{s1} \\ \hline \underline{\varepsilon}_{(m-s)1} \end{pmatrix} = \begin{pmatrix} W^{\frac{1}{2}} \cdot \underline{c} \\ \hline \omega^{\frac{1}{2}} \cdot \underline{\varepsilon} \end{pmatrix} \tag{16}$$

whilst in (7)

$$\overset{*}{W}^{\frac{1}{2}} \cdot \overset{*}{F} = \left(\begin{array}{c|c} \underset{ss}{W^{\frac{1}{2}}} & \underset{s(m-s)}{O} \\ \hline \underset{(m-s)s}{O} & \underset{(m-s)(m-s)}{\overset{*}{\omega}^{\frac{1}{2}}} \end{array}\right) \cdot \left(\begin{array}{c|c} \underset{st}{A} & \underset{s(n-t)}{\overset{*}{\beta}} \\ \hline \underset{(m-s)t}{\overset{*}{\gamma}} & \underset{(m-s)(n-t)}{\overset{*}{\alpha}} \end{array}\right) = \left(\begin{array}{c|c} W^{\frac{1}{2}} \cdot A & W^{\frac{1}{2}} \cdot \overset{*}{\beta} \\ \hline \overset{*}{\omega}^{\frac{1}{2}} \cdot \overset{*}{\gamma} & \overset{*}{\omega}^{\frac{1}{2}} \cdot \overset{*}{\alpha} \end{array}\right) \tag{17}$$

and

$$\overset{*}{W}^{\frac{1}{2}} \cdot \overset{*}{\underline{h}} = \left(\begin{array}{c|c} W^{\frac{1}{2}} & O \\ \hline O & \overset{*}{\omega}^{\frac{1}{2}} \end{array}\right) \cdot \left(\begin{array}{c} \underset{s1}{\underline{c}} \\ \hline \underset{(m-s)1}{\overset{*}{\underline{\varepsilon}}} \end{array}\right) = \left(\begin{array}{c} W^{\frac{1}{2}} \cdot \underline{c} \\ \hline \overset{*}{\omega}^{\frac{1}{2}} \cdot \overset{*}{\underline{\varepsilon}} \end{array}\right) \tag{18}$$

Bearing in mind that the * over a matrix or vector in (17) and (18) indicates a perturbed version of the corresponding matrix or vector in (15) and (16) without the * it is seen, comparing (17) with (15) and (18) with (16) that the motivation is to place the unchanged portions of the perturbed matrices in the upper left hand partitions and the unchanged portion of the perturbed $\underline{h}$ vector ($\underline{h}$) in the top part of the partitioned vector. Now if

$$\delta F = \overset{*}{F} - F \tag{19}$$

$$\delta\beta = \overset{*}{\beta} - \beta \tag{20}$$

$$\delta\gamma = \overset{*}{\gamma} - \gamma \tag{21}$$

$$\delta\omega = \overset{*}{\omega} - \omega \tag{22}$$

$$\delta\underline{\varepsilon} = \overset{*}{\underline{\varepsilon}} - \underline{\varepsilon} \tag{23}$$

then

$$\delta F = \left(\begin{array}{c|c} O & \delta\beta \\ \hline \delta\gamma & \delta\alpha \end{array}\right), \quad \delta W = \left(\begin{array}{c|c} O & O \\ \hline O & \delta\omega \end{array}\right), \quad \delta\underline{h} = \left(\begin{array}{c} \underline{O} \\ \hline \delta\underline{\varepsilon} \end{array}\right) \tag{24}$$

We also have

$$\delta Q = \overset{\sim}{\overset{*}{F}} \cdot \overset{*}{W} \cdot \overset{*}{F} - \tilde{F} \cdot W \cdot F \tag{25}$$

which can be expressed as

$$\delta Q = \overset{\sim}{\overset{*}{F}} \cdot \overset{*}{W} \cdot \delta F + \delta\tilde{F} \cdot W \cdot F + \overset{\sim}{\overset{*}{F}} \cdot \delta W \cdot F \tag{26}$$

Then by substituting term by term in (26) from (15), (17), and (24) we get

$$\delta Q = \left(\begin{array}{c|c} \tilde{A} & \tilde{\overset{*}{\gamma}} \\ \hline \tilde{\overset{*}{\beta}} & \tilde{\overset{*}{\alpha}} \end{array}\right) \cdot \left(\begin{array}{c|c} W & 0 \\ \hline 0 & \overset{*}{\omega} \end{array}\right) \cdot \left(\begin{array}{c|c} 0 & \delta\beta \\ \hline \delta\gamma & \delta\alpha \end{array}\right) + \left(\begin{array}{c|c} 0 & \delta\tilde{\gamma} \\ \hline \delta\tilde{\beta} & \delta\tilde{\alpha} \end{array}\right) \cdot \left(\begin{array}{c|c} W & 0 \\ \hline 0 & \omega \end{array}\right) \cdot \left(\begin{array}{c|c} A & \beta \\ \hline \gamma & \alpha \end{array}\right)$$

$$+ \left(\begin{array}{c|c} \tilde{A} & \tilde{\overset{*}{\gamma}} \\ \hline \tilde{\overset{*}{\beta}} & \tilde{\overset{*}{\alpha}} \end{array}\right) \cdot \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & \delta\omega \end{array}\right) \cdot \left(\begin{array}{c|c} A & \beta \\ \hline \gamma & \alpha \end{array}\right)$$

i.e.

$$\delta Q = \left(\begin{array}{c|c} \tilde{\overset{*}{\gamma}} & \delta\tilde{\gamma} \\ \hline \tilde{\overset{*}{\alpha}} & \delta\alpha \end{array}\right) \cdot \left(\begin{array}{c|c} \overset{*}{\omega} \cdot \delta\gamma & \overset{*}{\omega} \cdot \delta\alpha \\ \hline \omega \cdot \gamma & \omega \cdot \alpha \end{array}\right) + \left(\begin{array}{c|c} 0 & \tilde{A} \\ \hline \delta\tilde{\beta} & \tilde{\overset{*}{\beta}} \end{array}\right) \cdot \left(\begin{array}{c|c} W \cdot A & W \cdot \beta \\ \hline 0 & W \cdot \delta\beta \end{array}\right)$$

$$+ \left(\begin{array}{c} \tilde{\overset{*}{\gamma}} \\ \hline \tilde{\overset{*}{\alpha}} \end{array}\right) \cdot \delta\omega \cdot \left(\begin{array}{c|c} \gamma & \alpha \end{array}\right)$$

which is the same as

$$\delta Q = \left(\begin{array}{c|c} \tilde{\overset{*}{\gamma}} & \tilde{\delta\gamma} \\ \hline \tilde{\overset{*}{\alpha}} & \tilde{\delta\alpha} \end{array}\right) \cdot \left(\begin{array}{c|c} \overset{*}{\omega} & 0 \\ \hline 0 & \omega \end{array}\right) \cdot \left(\begin{array}{c|c} \delta\gamma & \delta\alpha \\ \hline \gamma & \alpha \end{array}\right)$$

$$+ \left(\begin{array}{c|c} 0 & \tilde{A} \\ \hline \tilde{\delta\beta} & \tilde{\overset{*}{\beta}} \end{array}\right) \cdot \left(\begin{array}{c|c} W & 0 \\ \hline 0 & W \end{array}\right) \cdot \left(\begin{array}{c|c} A & \beta \\ \hline 0 & \delta\beta \end{array}\right)$$

$$+ \left(\begin{array}{c} \tilde{\overset{*}{\gamma}} \\ \hline \tilde{\overset{*}{\alpha}} \end{array}\right) \cdot \delta\omega \cdot \left(\begin{array}{c|c} \gamma & \alpha \end{array}\right) \qquad (27)$$

Similarly we have that

$$\delta\underline{\ell} = \underline{\ell}^{*} - \underline{\ell} = \tilde{F}^{*} \cdot W^{*} \cdot \underline{h}^{*} - \tilde{F} \cdot W \cdot \underline{h}$$

i.e.

$$\delta\underline{\ell} = \tilde{F}^{*} \cdot W^{*} \cdot \delta\underline{h} + \delta\tilde{F} \cdot W \cdot \underline{h} + \tilde{F}^{*} \cdot \delta W \cdot \underline{h} \qquad (28)$$

and now, using (28) and (24) we get

$$\delta\underline{\ell} = \begin{pmatrix} \tilde{A} & \tilde{\gamma}^{*} \\ \tilde{\beta}^{*} & \tilde{\alpha} \end{pmatrix} \cdot \begin{pmatrix} W & 0 \\ 0 & \omega^{*} \end{pmatrix} \cdot \begin{pmatrix} \underline{o} \\ \delta\underline{\varepsilon} \end{pmatrix} + \begin{pmatrix} 0 & \delta\tilde{\gamma} \\ \delta\tilde{\beta} & \delta\tilde{\alpha} \end{pmatrix} \cdot \begin{pmatrix} W & 0 \\ 0 & \omega \end{pmatrix} \cdot \begin{pmatrix} \underline{c} \\ \underline{\varepsilon} \end{pmatrix}$$

$$+ \begin{pmatrix} \tilde{A} & \tilde{\gamma}^{*} \\ \tilde{\beta}^{*} & \tilde{\alpha} \end{pmatrix} \cdot \begin{pmatrix} 0 & 0 \\ 0 & \delta\omega \end{pmatrix} \cdot \begin{pmatrix} \underline{c} \\ \underline{\varepsilon} \end{pmatrix}$$

which re-orders to

$$\delta\underline{\ell} = \begin{pmatrix} \tilde{\gamma}^{*} & \delta\tilde{\gamma} \\ \tilde{\alpha}^{*} & \delta\tilde{\alpha} \end{pmatrix} \cdot \begin{pmatrix} \omega^{*} & 0 \\ 0 & \omega \end{pmatrix} \cdot \begin{pmatrix} \delta\underline{\varepsilon} \\ \underline{\varepsilon} \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ \delta\tilde{\beta} & 0 \end{pmatrix} \cdot \begin{pmatrix} W & 0 \\ 0 & W \end{pmatrix} \cdot \begin{pmatrix} \underline{c} \\ \underline{o} \end{pmatrix}$$

$$+ \begin{pmatrix} \tilde{\gamma}^{*} \\ \tilde{\alpha}^{*} \end{pmatrix} \cdot \delta\omega \cdot \underline{\varepsilon}$$

and to make this correspond more closely to (27) it may be written as

$$\delta\underline{\ell} = \begin{pmatrix} \tilde{\gamma}^{*} & \delta\tilde{\gamma} \\ \tilde{\alpha}^{*} & \delta\tilde{\alpha} \end{pmatrix} \cdot \begin{pmatrix} \omega^{*} & 0 \\ 0 & \omega \end{pmatrix} \cdot \begin{pmatrix} \delta\underline{\varepsilon} \\ \underline{\varepsilon} \end{pmatrix} + \begin{pmatrix} 0 & \tilde{A} \\ \delta\tilde{\beta} & \tilde{\beta}^{*} \end{pmatrix} \cdot \begin{pmatrix} W & 0 \\ 0 & W \end{pmatrix} \cdot \begin{pmatrix} \underline{c} \\ \underline{o} \end{pmatrix} + \begin{pmatrix} \tilde{\gamma}^{*} \\ \tilde{\alpha}^{*} \end{pmatrix} \cdot \delta\omega \cdot \underline{\varepsilon} \qquad (29)$$

Now if we put

$$K = \begin{pmatrix} \tilde{\gamma}^{*} & \delta\tilde{\gamma} \\ \tilde{\alpha}^{*} & \delta\tilde{\alpha} \end{pmatrix} \quad , \quad J = \begin{pmatrix} 0 & \tilde{A} \\ \delta\tilde{\beta} & \tilde{\beta}^{*} \end{pmatrix} \qquad (30)$$

Now if we put

$$K = \begin{pmatrix} \tilde{\gamma}^* & \delta\tilde{\gamma} \\ \tilde{\alpha}^* & \delta\tilde{\alpha} \end{pmatrix} \quad , \quad J = \begin{pmatrix} 0 & \tilde{A} \\ \delta\tilde{\beta} & \tilde{\beta}^* \end{pmatrix} \tag{30}$$

then from (13), (27) and (29) there follows the required expression for the perturbation $\delta\underline{a}$ in the coefficient vector

$$\delta\underline{a} = Q^{*-1} \cdot \left\{ K \cdot \begin{pmatrix} \omega^* & 0 \\ 0 & \omega \end{pmatrix} \cdot \begin{pmatrix} \delta\underline{\varepsilon} \\ \underline{\varepsilon} \end{pmatrix} + J \cdot \begin{pmatrix} W & 0 \\ 0 & W \end{pmatrix} \cdot \begin{pmatrix} \underline{c} \\ \underline{o} \end{pmatrix} + \begin{pmatrix} \tilde{\gamma}^* \\ \tilde{\alpha}^* \end{pmatrix} \cdot \delta\omega \cdot \underline{\varepsilon} \right.$$

$$\left. - \left[ K \cdot \begin{pmatrix} \omega^* & 0 \\ 0 & \omega \end{pmatrix} \cdot \begin{pmatrix} \delta\gamma & \delta\alpha \\ \gamma & \alpha \end{pmatrix} + J \cdot \begin{pmatrix} W & 0 \\ 0 & W \end{pmatrix} \cdot \begin{pmatrix} A & \beta \\ 0 & \delta\beta \end{pmatrix} + \begin{pmatrix} \tilde{\gamma}^* \\ \tilde{\alpha}^* \end{pmatrix} \cdot \delta\omega \cdot (\gamma \mid \alpha) \right] \cdot \underline{a} \right\} \tag{31}$$

or, otherwise expressed

$$\delta\underline{a} = Q^{*-1} \cdot \left\{ K \cdot \begin{pmatrix} \omega^* & 0 \\ 0 & \omega \end{pmatrix} \cdot \left[ \begin{pmatrix} \delta\underline{\varepsilon} \\ \underline{\varepsilon} \end{pmatrix} - \begin{pmatrix} \delta\gamma & \delta\alpha \\ \gamma & \alpha \end{pmatrix} \cdot \underline{a} \right] \right.$$

$$+ J \cdot \begin{pmatrix} W & 0 \\ 0 & W \end{pmatrix} \cdot \left[ \begin{pmatrix} \underline{c} \\ \underline{o} \end{pmatrix} - \begin{pmatrix} A & \beta \\ 0 & \delta\beta \end{pmatrix} \cdot \underline{a} \right] \tag{32}$$

$$\left. + \begin{pmatrix} \tilde{\gamma}^* \\ \tilde{\alpha}^* \end{pmatrix} \cdot \delta\omega \cdot \left[ \underline{\varepsilon} - (\gamma \mid \alpha) \cdot \underline{a} \right] \right\}$$

Instead of (13), (27) and (29) we could use (14), (27) and (29) to get

$$\delta\underline{a} = Q^{-1} \cdot \left\{ K \cdot \begin{pmatrix} \omega^* & 0 \\ 0 & \omega \end{pmatrix} \cdot \left[ \begin{pmatrix} \delta\underline{\varepsilon} \\ \underline{\varepsilon} \end{pmatrix} - \begin{pmatrix} \delta\gamma & \delta\alpha \\ \gamma & \alpha \end{pmatrix} \cdot \overset{*}{\underline{a}} \right] \right.$$

$$+ J \cdot \begin{pmatrix} W & 0 \\ 0 & W \end{pmatrix} \cdot \left[ \begin{pmatrix} \underline{c} \\ \underline{o} \end{pmatrix} - \begin{pmatrix} A & \beta \\ 0 & \delta\beta \end{pmatrix} \cdot \overset{*}{\underline{a}} \right] \tag{33}$$

$$\left. + \begin{pmatrix} \tilde{\gamma}^* \\ \tilde{\alpha}^* \end{pmatrix} \cdot \delta\omega \cdot \left[ \underline{\varepsilon} - (\gamma \mid \alpha) \cdot \overset{*}{\underline{a}} \right] \right\}$$

Either or both of the expressions (32) and (33) may now be used to study the many special cases which turn up in practice. One or two such special cases may be discussed in further Notes on this topic.

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